

#Ligand	TotalEnergy	VDW	AverConPair
model1_7b3d-Roccustyrna_fr1-0.pdb	-930.007	-930.007	986.957
model1_7b3d-Roccustyrna_fr2-0.pdb	-922.901	-922.901	185.758
model1_7b3d-Darunavir_CID_213039-0.pdb	-921.521	-921.521	162.632
model1_7b3d-Merimepodib_CID_153241-0.pdb	-885.756	-885.756	176.667
model1_7b3d-GissitorviffirnaTM8-0.pdb	-866.098	-866.098	142.105
model1_7b3d-Roccustyrna_fr6-0.pdb	-860.395	-860.395	145.789
model1_7b3d-GissitorviffirnaTM9-0.pdb	-838.754	-838.754	156.471
model1_7b3d-Amprenavir_CID_65016-0.pdb	-804.653	-804.653	147.143
model1_7b3d-GissitorviffirnaTM7-0.pdb	-784.015	-784.015	146.842
model1_7b3d-Indinavir_CID_5362440-0.pdb	-778.624	-778.624	129.333
model1_7b3d-Roccustyrna_fr4-0.pdb	-759.032	-759.032	149.722
model1_7b3d-Roccustyrna_gs2-0.pdb	-753.732	-753.732	258.421
model1_7b3d-Vidarabine_CID_21704-0.pdb	-747.682	-747.682	282.105
model1_7b3d-Asunaprevir_CID_16076883-0.pdb	-718.509	-718.509	129.216
model1_7b3d-Taribavirin_CID_451448-0.pdb	-693.734	-693.734	272.941
model1_7b3d-Penciclovir_CID_135398748-0.pdb	-664.803	-664.803	258.333
model1_7b3d-Galidesivir_CID_10445549-0.pdb	-660.762	-660.762	265.263
model1_7b3d-Maribavir_CID_471161-0.pdb	-653.666	-653.666	169.583
model1_7b3d-Zanamivir_CID_60855-0.pdb	-643.364	-643.364	205.217
model1_7b3d-GissitorviffirnaTM4-0.pdb	-642.045	-642.045	20.55
model1_7b3d-Tenofovir_CID_464205-0.pdb	-634.657	-634.657	289.474
model1_7b3d-Roccustyrna_gs6-0.pdb	-626.317	-626.317	21.2
model1_7b3d-GissitorviffirnaTM1-0.pdb	-606.768	-606.768	169.545
model1_7b3d-Cytarabine_CID_6253-0.pdb	-602.039	-602.039	227.647
model1_7b3d-Faldaprevir_CID_42601552-0.pdb	-411.564	-411.564	761.404
model1_7b3d-Famciclovir_CID_3324-0.pdb	-244.602	-244.602	131.304
model1_7b3d-Roccustyrna_gs5-0.pdb	-103.093	-103.093	523.438
model1_7b3d-Boceprevir_CID_10324367-0.pdb	61.156	61.156	137.568
model1_7b3d-Roccustyrna_fr5-0.pdb	124.914	124.914	109.412
model1_7b3d-Roccustyrna_fr3-0.pdb	129.971	129.971	188.718
model1_7b3d-Atazanavir_CID_148192-0.pdb	155.715	155.715	492.157
model1_7b3d-Sofosbuvir_CID_45375808-0.pdb	229.342	229.342	239.722
model1_7b3d-Valganciclovir_CID_135413535-0.pdb	239.644	239.644	20.12
model1_7b3d-Nelfinavir_CID_64143-0.pdb	258.344	258.344	11.35
model1_7b3d-Ritonavir_CID_392622-0.pdb	338.039	338.039	7.44
model1_7b3d-GissitorviffirnaTM6-0.pdb	419.377	419.377	152.308
model1_7b3d-Lopinavir_CID_92727-0.pdb	514.324	514.324	162.391
model1_7b3d-Roccustyrna_gs3-0.pdb	526.744	526.744	199.149
model1_7b3d-Roccustyrna_gs4-0.pdb	624.329	624.329	106.078
model1_7b3d-Sorivudine_CID_5282192-0.pdb	647.168	647.168	18.55
model1_7b3d-Roccustyrna_gs8-0.pdb	834.743	834.743	22.64
model1_7b3d-Roccustyrna_gs1-0.pdb	317.78	317.78	148.261
model1_7b3d-Roccustyrna_fr7-0.pdb	-80.61	-80.61	188.286